

Supporting Information

The investigation on the structural, optical, photoluminescence and electric properties in a semiconductor material $[\text{Br}(\text{CH}_2)_2\text{N}(\text{CH}_3)_3]_2\text{SnBr}_6$

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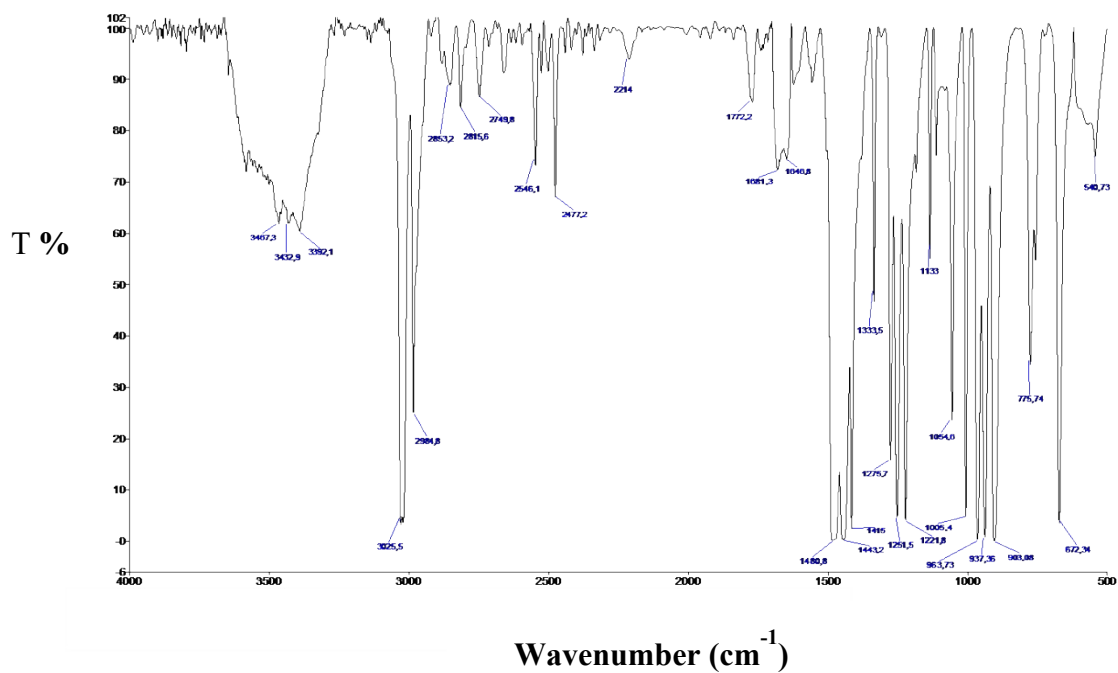


Figure S1: Infrared absorption spectrum of the compound $[\text{Br}(\text{CH}_2)_2\text{N}(\text{CH}_3)_3]_2\text{SnBr}_6$.

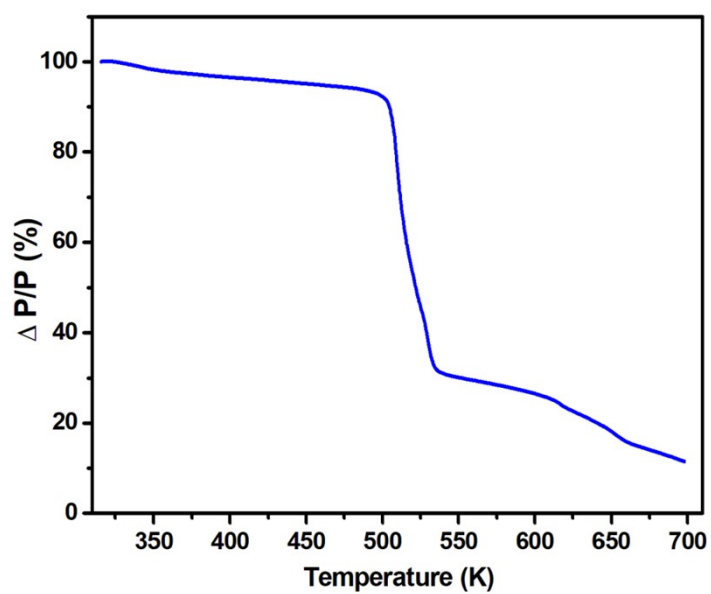


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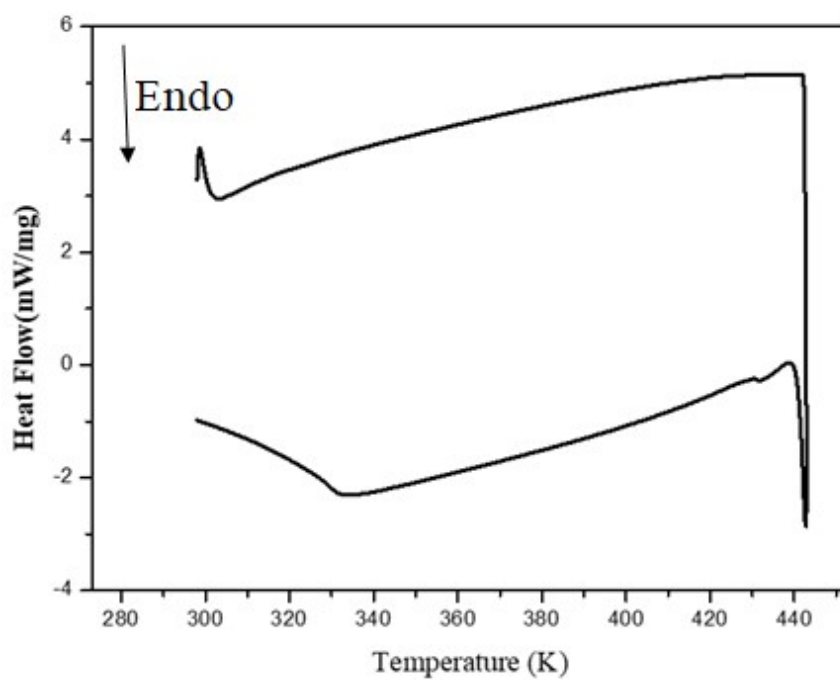


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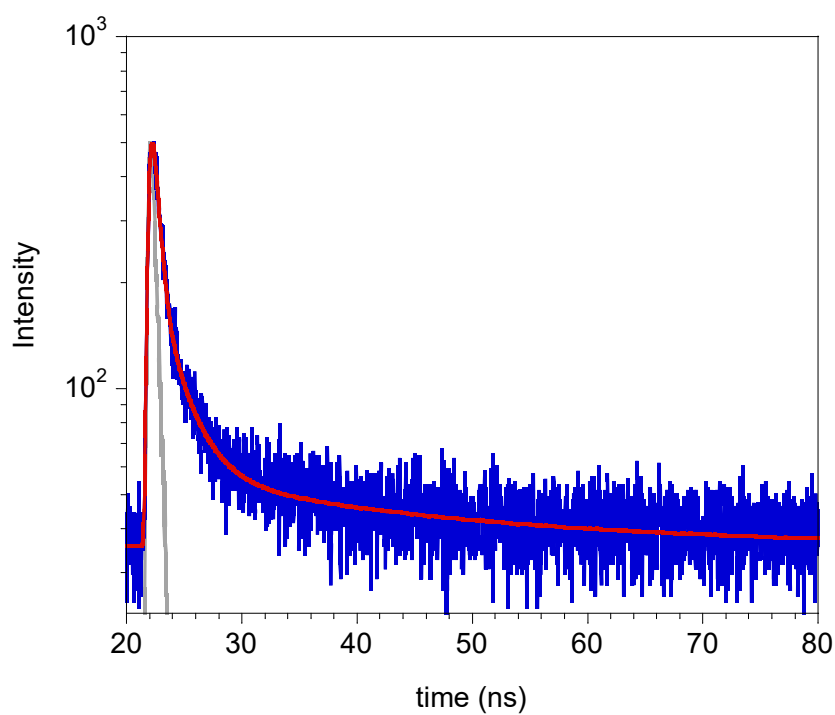


Figure S4: PL decay of $[\text{Br}(\text{CH}_2)_2\text{N}(\text{CH}_3)_3]_2\text{SnBr}_6$ powders. Excitation 300nm Three exponential fit (red line) with parameters: $t_1 = 2.2215\text{E-}09$ sec ; $t_2 = 2.314715\text{E-}08$ sec ; $t_3 = 2.328581\text{E-}10$ sec ; $A_1 = 1.090455\text{E-}02$; $A_2 = 1.492454\text{E-}03$; $A_3 = 0.117697$; CHISQ = 1.208462.

$$\text{Average lifetime is } \langle t \rangle = \sum_i \frac{A_i \tau_i}{A_i} = 662\text{ps}$$

Table S1. Crystallographic data and structure refinement parameters for $[\text{Br}(\text{CH}_2)_2\text{N}(\text{CH}_3)_3]_2\text{SnBr}_6$.

Chemical formula	$[\text{C}_5\text{H}_{13}\text{NBr}]_2\text{SnBr}_6$
Molecular weight (g/mol)	932.30
Crystal system	Orthorhombic
Space group	<i>Pbca</i>
a (Å)	12.792 (2)
b (Å)	12.973 (2)
c (Å)	14.605 (2)
Volume (Å ³)	2423.7 (6)
Z	4
Temperature (K)	150
Crystal dimensions (mm ³)	0.050 × 0.070 × 0.130
Crystal color	Colorless
Linear absorption coefficient (mm ⁻¹)	14.24
Radiation (λ, Å)	0.71073 (MoKα)
Density Dx (Mg/m ³)	2.555
Absorption correction	Multi-scan
Measured reflections	20567
Independent reflections	2786
Reflections [I > 2σ(I)]	2332
Measurement range (h, k, l)	-16 ≤ h ≤ 16 ; -16 ≤ k ≤ 16; -18 ≤ l ≤ 17
No. of refined parameters	98
R ₁	0.020
wR ₂	0.035
Goodness-of-fit (GoF)	1.03
F(000)	1720

Table S2. Selected bond distances (Å) and angles (°) for [Br(CH₂)₂N(CH₃)₃]₂SnBr₆.

Distances (Å)		Angles (°)	
Sn—Br1	2.5587 (5)	Br1—Sn—Br1 ⁽ⁱ⁾	180.0
Sn—Br1 ⁽ⁱ⁾	2.5587 (5)	Br1—Sn—Br2	90.888 (11)
Sn—Br2	2.6156 (5)	Br1 ⁽ⁱ⁾ —Sn—Br2	89.112 (11)
Sn—Br2 ⁽ⁱ⁾	2.6156 (5)	Br1—Sn—Br3	89.451 (9)
Sn—Br3	2.6070 (4)	Br1 ⁽ⁱ⁾ —Sn—Br3	90.548 (9)
Sn—Br3 ⁽ⁱ⁾	2.6070 (4)	Br1—Sn—Br3 ⁽ⁱ⁾	90.549 (9)
		Br1 ⁽ⁱ⁾ —Sn—Br3 ⁽ⁱ⁾	89.452 (9)
		Br3—Sn—Br3 ⁽ⁱ⁾	180.0
		Br3—Sn—Br2	89.889 (10)
		Br3 ⁽ⁱ⁾ —Sn—Br2	90.111 (10)
		Br1—Sn—Br2 ⁽ⁱ⁾	89.112 (11)
		Br3—Sn—Br2 ⁽ⁱ⁾	90.111 (10)
		Br3 ⁽ⁱ⁾ —Sn—Br2 ⁽ⁱ⁾	89.889 (10)
		Br2—Sn—Br2 ⁽ⁱ⁾	180.0
		Br1 ⁽ⁱ⁾ —Sn—Br2 ⁽ⁱ⁾	90.888 (11)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Table S3. Selected bond distances (Å) and angles (°) in the organic framework of $[\text{Br}(\text{CH}_2)_2\text{N}(\text{CH}_3)_3]_2\text{SnBr}_6$.

Distances (Å)		Angles (°)	
Br4—C1	1.943 (3)	C3—N1—C4	108.7 (2)
N1—C3	1.489 (4)	C3—N1—C5	110.1 (2)
N1—C4	1.500 (4)	C4—N1—C5	108.4 (2)
N1—C5	1.504 (3)	C3—N1—C2	111.1 (2)
N1—C2	1.511 (4)	C4—N1—C2	107.1 (2)
C2—C1	1.502 (4)	C5—N1—C2	111.3 (2)
		C1—C2—N1	114.4 (2)
		C2—C1—Br4	108.8 (2)

Table S4 : Hydrogen-bonding geometry (Å, °) for $[\text{Br}(\text{CH}_2)_2\text{N}(\text{CH}_3)_3]_2\text{SnBr}_6$.

$D\text{—H}\cdots A$	$D\text{—H}$	$\text{H}\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
C2—H2A \cdots Br3 ⁽ⁱⁱ⁾	0.99	3.10	3.995 (3)	151
C2—H2B \cdots Br3 ⁽ⁱ⁾	0.99	3.13	3.984 (3)	145
C5—H5B \cdots Br1	0.98	3.10	3.669 (3)	118
C5—H5B \cdots Br3 ⁽ⁱ⁾	0.98	2.85	3.784 (3)	160
C5—H5C \cdots Br3 ⁽ⁱⁱⁱ⁾	0.98	2.87	3.830 (3)	168
C5—H5A \cdots Br2 ^(iv)	0.98	2.98	3.913 (3)	160
C4—H4A \cdots Br1 ⁽ⁱⁱ⁾	0.98	3.02	3.920 (3)	153
C4—H4C \cdots Br1 ⁽ⁱⁱⁱ⁾	0.98	3.03	3.883 (3)	146
C3—H3A \cdots Br3 ^(v)	0.98	3.10	3.896 (3)	140
C3—H3B \cdots Br1 ⁽ⁱⁱ⁾	0.98	2.90	3.829 (3)	158

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, -y+3/2, z-1/2$; (iii) $-x+3/2, -y+1, z-1/2$; (iv) $-x+3/2, y+1/2, z$; (v) $x+1/2, -y+3/2, -z+1$.